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Determination of the Self-Compensation Ratio of Carbon in AlGaN for HEMTs

Ben Rackauskas, Michael J. Uren, *Member, IEEE*, Steve Stoffels, Ming Zhao, Stefaan Decoutere, and Martin Kuball, *Senior Member, IEEE*

***Abstract*— Epitaxial AlGaN/GaN/AlGaN-on-Si high-electron mobility structures with and without carbon doping have been studied. By considering the donor density required to suppress a 2D hole gas in the undoped structure, we demonstrate that the 2×10^{19} cm^{-3} substitutional carbon incorporated during metal-organic chemical vapor deposition must be a source of donors as well as acceptors, with a donor to acceptor ratio of at least 0.4. This compensation ratio was determined based on the comparison of substrate bias experiments with TCAD simulations. This value, which was previously unknown, is a key parameter in GaN power switching high- electron-mobility transistors, since it determines the resistivity of the layer used to suppress leakage and increase breakdown voltage.**

***Index Terms*— 2D hole gas (2DHG), AlGaN, carbon, GaN, compensation, self-compensation.**

I. Introduction

GALLIUM nitride is a key material system for efficient, high-power electronic devices. In AlGaN/GaN high-electron-mobility transistors, carbon is not only inevitably present in low densities as an unintentional dopant [1] but often also intentionally incorporated in high densities to suppress buffer conduction and increase breakdown voltage [2], [3]. However, despite this, there is still much debate and considerable confusion about the way in which high densities of carbon incorporate into (Al)GaN during metal-organic chemical vapor deposition growth [4]–[6]. Current theoretical results suggest that the key levels for substitutional carbon are an acceptor state for the nitrogen site (C_N) with a level of $E_V + 0.9$ eV for GaN increasing to $E_V + 1.88$ eV for AlN [5]–[7], and a donor state in or near the conduction band for the Ga site in GaN (C_{Ga}) or Al site in AlN. This C_N level correlates with spectroscopic data [8]–[10] and electrical measurements [11].

When incorporated in GaN or AlGaN-on-Si devices in high concentrations (i.e., $>10^{18}$ cm^{-3}), the compensation ratio (donor/acceptor density, N_d/N_a) of carbon is important since it, and not the carbon density alone, determines the free carrier density, and thus the resistivity and bulk leakage [12], [13]. This is not necessarily the case at low (unintentional) concentrations where other carbon levels may be more important [14]. Unfortunately at present, there are no direct measurements of the carbon self-compensation ratio, although indirect measurements of resistivity do suggest the C_N level is compensated with ratios of 0.1–0.6 [15]. Recent electrical measurements have directly demonstrated that the Fermi level is pinned near the C_N acceptor level in heavily carbon-doped GaN demonstrating that C_N is dominant [16], consistent with the predictions of Lyons *et al.* [5]. However, this paper did not give an indication of the compensation ratio. This paper considers AlGaN with 8% Al and provides strong evidence that the carbon density of 2×10^{19} cm^{-3} is electrically active, primarily substituted on the nitrogen site as an acceptor but also highly compensated with a donor density of at least 5×10^{18} cm^{-3}. It seems entirely reasonable that this high donor density is largely due to carbon self-compensating and substituting on the (Al)Ga site as a shallow donor.

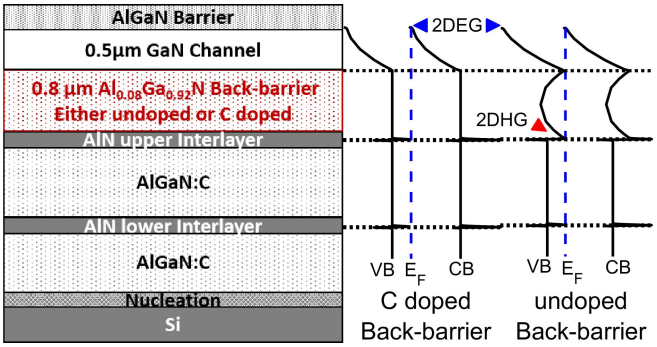

Fig. 1. Schematic epitaxy of the two studied samples is shown together with simulated band diagrams with no applied bias. The 2DHG (indicated above the upper interlayer) is present only in the undoped sample.

II. Experimental Details

Two epitaxial structures were studied, with the structure schematic shown in Fig. 1, with a 0.8 μm $Al_{0.08}Ga_{0.92}N$ back barrier. Both were grown with nominally identical structure except for the doping in the $Al_{0.08}Ga_{0.92}N$ back barrier, which

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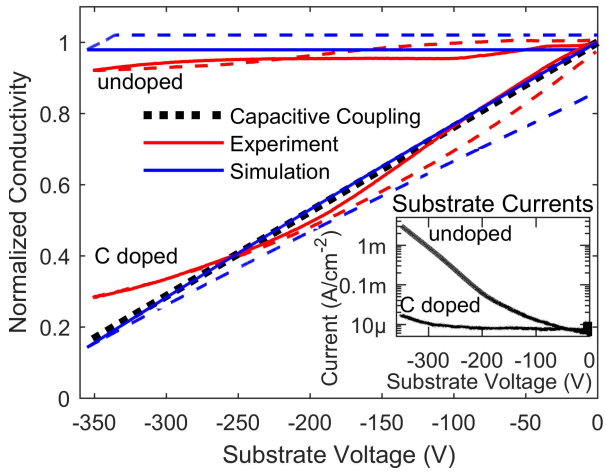

Fig. 2. Experimental and simulated 2DEG conductivity as the Si back-bias is ramped with, inset, the substrate currents during the measurement. The solid line corresponds to the downward sweep and the dashed line the return to 0 V, both at a rate of 5 V/s. The capacitive coupling line corresponds to the expected response of an ideal dielectric buffer.

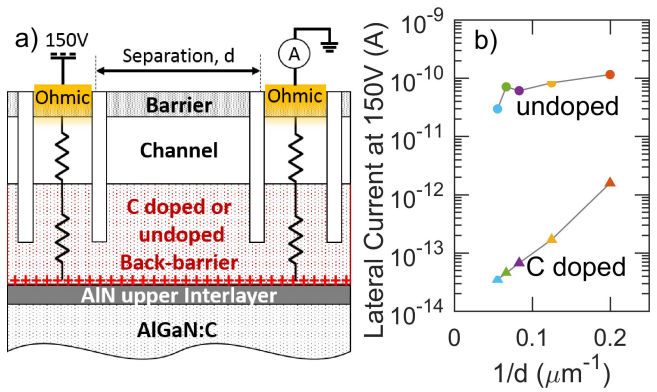

Fig. 3. (a) Isolation structure used in the lateral leakage measurements with an equivalent circuit diagram overlaid. The leakage current with 150 V between the contacts for the undoped and carbon doped samples is shown in (b). The lateral leakage in the undoped sample was very weakly dependent on contact separation indicating a low resistance lateral conduction path, consistent with the presence of a 2DHG.

was either undoped or carbon doped with a concentration of $\sim 2 \times 10^{19}$ cm^{-3} as measured by secondary ion mass spectroscopy. The resulting simulated band diagrams are also shown (discussed later).

The back-bias technique was applied on an ungated 20-μm ohmic-to-ohmic contact gap TLM structure and used to assess vertical charge transport within the epitaxy. The technique monitors the conductivity of the 2D electron gas (2DEG), while a ramped substrate bias is applied. The 2DEG current is measured with one ohmic at 1 V and the other at 0 V. If the 2DEG is never pinched off, the surface does not experience any strong electric fields. Consequently, this technique ensures the channel conductivity is influenced only by buffer related effects. More details on the technique can be found in [15] and [17]–[19].

III. Results and Discussion

Fig. 2 shows the result of a substrate ramp experiment for the two samples. In the carbon-doped sample, the 2DEG density depleted roughly linearly with applied negative substrate bias, very close to that expected for back-gating, if the epitaxial stack were behaving as an insulating dielectric layer (black dashed line). This indicates a linear potential drop vertically across the stack, consistent with previous back-bias studies of carbon-doped GaN layers [15], although in this paper, we studied 8% AlGaN. In contrast, the 2DEG density in the undoped sample was only very weakly dependent on the substrate bias indicating that the majority of the potential was dropped over the lower part of the stack. From electrostatics, this must be caused by the accumulation of positive charge in the stack with the effect of reducing the vertical field in the channel. The higher substrate current in the undoped sample is consistent with an increased vertical field through the strain relief layers.

Such screening behavior in the undoped sample requires a positively charged layer in the buffer whose density can vary in response to the applied field and span, at least, the area between the contacts. A reasonable inference is that a polarization-induced 2D hole gas (2DHG) forms above the upper interlayer [20]–[24] (indicated in the undoped band diagram of Fig. 1) which is electrically in contact with the ohmic contacts, allowing its density to change with substrate bias. One possible mechanism for this electrical contact is via extended defects as suggested previously [25]. A possible alternative explanation for the screening would be a population of donors in the undoped back barrier [26]. However, screening has been demonstrated up to -600 V, requiring a donor density $>1.3 \times 10^{17}$ cm^{-3} assuming uniform distribution throughout the back barrier. Such a high donor density seems unlikely in a good quality UID layer. Conversely, the linear depletion of the 2DEG with bias in the carbon-doped sample implies the hole gas is not present but suppressed by the carbon incorporation. Polarization-induced 2DHG formation has been observed in the past and suppressed by the intentional incorporation of donors [14], [27].

To examine the impact of a 2DHG, lateral leakage was measured between two 100×100 μm contacts both surrounded by a mesa etch, which extended down to part way through the back barrier, as shown in Fig. 3(a). This isolated the 2DEG but allowed a 2DHG (if present) to act as deep lateral conduction path between the two contacts. A bias was applied between the contacts with the resulting lateral leakage shown in Fig. 3(b). In the carbon-doped sample, the leakage current decreased exponentially with increasing separation, as would be expected for a field dependent leakage by a process such as variable range hopping [28]. However, in the undoped sample, the leakage current remained high and was broadly gap independent. Assuming the equivalent circuit diagram overlaid in Fig. 3(a), separation independence is consistent with a low lateral resistance compared to the two vertical paths. Though this cannot be viewed as proof, it is consistent with the assertion that a 2DHG is present in only the undoped sample.

Here, we aim to use the suppression of the 2DHG by carbon doping to set limits on the donor density, and hence the

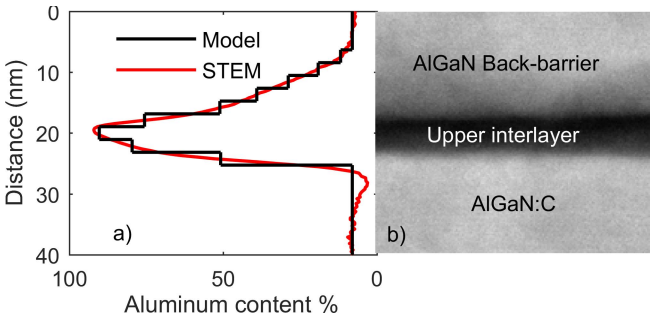

Fig. 4. Composition profile of the interlayers from an STEM cross section and the model used in this simulation are shown in (a) with the raw STEM image shown in (b).

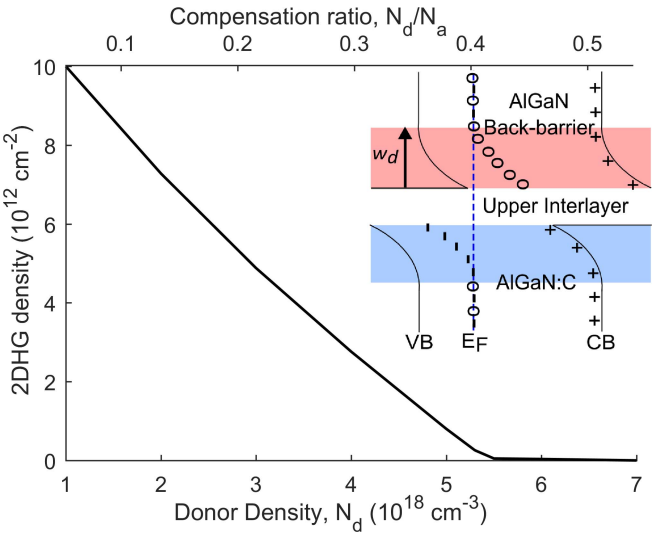

Fig. 5. Number of C_{AlGa} (donor density) required to suppress the formation of a 2DHG at the upper interlayer when carbon doped. Inset is a sketch of the band diagram which demonstrates how ionized donors are exposed in the depletion region (of width w_d and shaded red) above the interlayers. The simulated depletion width ranged from 45 to 20 nm with donor densities of 1×10^{18} cm^{-3} and 6×10^{18} cm^{-3}, respectively.

compensation ratio. By comparing the substrate-bias results with TCAD simulations and tuning the compensation ratio in the simulation of the carbon-doped structure, it is possible to determine the minimum carbon self-compensation required to suppress the 2DHG. To do this, Silvaco's ATLAS 2-D drift-diffusion simulator was used; this allowed us to model the polarization-induced charge at the interlayers and the 2DHG formation. We assumed complete relaxation of the interlayers; this may result in a slight underestimate of the interface charge, if the layer is not fully relaxed. The interlayer composition was modeled based on a profile provided by a scanning transmission electron microscope (STEM) image acquired with a high-angle annular dark-field detector and is shown in Fig. 4.

The total carbon concentration was incorporated as a shallow donor (N_d) close to E_c corresponding to C_{Al} and C_{Ga} (denoted as C_{AlGa} here), and as a deep acceptor (N_a) at $E_v + 0.98$ eV corresponding to C_N [5], with a total density of $N_d + N_a = 2 \times 10^{19}$ cm^{-3}. This C_N level was evaluated from a linear interpolation between the C_N levels in GaN and AlN ($E_v + 0.9$ eV and $E_V + 1.88$ eV, respectively) for 8% AlGaN. In addition, 10^{16} cm^{-3} shallow donors were incorporated corresponding to a typical unintentional dopant density. The compensation ratio (N_d/N_a) of the carbon was varied to fit to the experimental data. The AlGaN top barrier surface charge was set to 5×10^{12} cm^{-2} to bring the simulated 2DEG density in line with Hall measurements of 5.9×10^{12} cm^{-2} and 50 nm p++ spikes were included under the contacts to allow charge injection as in [25].

In the simulation for the undoped AlGaN back barrier, a 2DHG formed with a density of 8×10^{12} cm^{-2} at the bottom of the back barrier. To simulate the carbon-doped AlGaN back barrier, carbon traps were included with compensation ratios ranging from 0.05 to 0.5. In this simulation of the carbon-doped structure, the 2DHG density, shown in Fig. 5, decreased with increasing compensation, i.e., fraction of carbon on the (Al)Ga site. To suppress the 2DHG by carbon doping the back barrier, as seen in the experiment, more than $\sim 5.5 \times 10^{18}$ cm^{-3} donors were required. This implies a compensation ratio of $N_d/N_a \geq 0.4$. Although increasing the compensation ratio reduces the acceptor density, as $N_d/N_a < 1$, this will only reduce the population of neutral acceptors which can vary without impact on the charge. The substrate bias ramps of both samples were simulated with $N_d/N_a = 0.4$ for the carbon-doped back-barrier and no carbon for the undoped back barrier. The simulation results, in Fig. 2, show good qualitative agreement with the measurements, showing that the 2DHG can indeed explain this behavior.

Suppression of the 2DHG, therefore, requires a population of donors, i.e., carbon on the (Al)Ga site. In the depletion region above the upper interlayer, depicted in the inset in Fig. 5, the Fermi level is lower than the C_N deep acceptor level. This means that the deep acceptor level is neutral and the ionized shallow donors are revealed, resulting in a positive space charge. At a sufficient donor density, this positive space-charge region completely neutralizes the negative polarization charge and suppresses the 2DHG. Only the donors can suppress the 2DHG and the density required here is in agreement with [14], though the source of donors there is different.

The results obtained here suggest the compensation ratio of carbon in these wafers to be $\geq$0.4. However, this is under the assumption that all the donors in the carbon-doped back barrier are $C_{(Al)Ga}$. This assumption may not be entirely correct, as to incorporate carbon requires changes to the growth conditions which will increase the density of other point defect donors such as nitrogen vacancies [29] (though in densities much lower than the 5.5×10^{18} cm^{-3} seen here).

This result of self-compensation is consistent with density functional theory calculations which show that the formation energy of substitutional carbon defects is strongly dependent on the position of the Fermi level during growth [5], [6]. As the Fermi level is in turn dependent on the site of the carbon incorporation (C_N acceptor or $C_{(Al)Ga}$ donor), the result is self-compensation at equilibrium during growth. A similar compensation ratio would be expected for pure GaN based on this result. Plausible reasons why carbon is not perfectly

self-compensating are kinetic effects and simultaneous incorporation of hydrogen also effecting the Fermi level during growth [5].

IV. Conclusion

The electrical behavior of two wafers, differing only by carbon doping in the $Al_{0.08}Ga_{0.92}N$ back barrier, has been measured and compared to models. The results suggest that the carbon incorporated in low Al percentage AlGaN at high densities is self-compensating with both C_N and $C_{(Al)Ga}$ present and, assuming an insignificant density of other point defect donors, a compensation ratio greater than 0.4 and less than 1. This previously unknown result has important consequences for carbon-doped GaN RF or power devices since it determines important device properties such as the bulk resistivity and the depletion behavior under the gate when pinched off. A reasonable estimate of compensation is a requirement for accurate device simulation.

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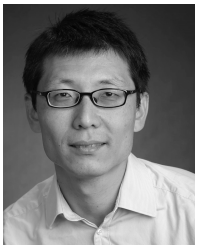

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